p-Isopropylbenzylamine

Other names: Benzylamine, p-isopropyl-,
Inchi: InChI=1S/C10H15N/c1-8(2)10-5-3-9(7-11)4-6-10/h3-6,8H,7,11H2,1-2H3
InchiKey: YQSHYGCCYVPRDI-UHFFFAOYSA-N
Formula: C10H15N
SMILES: CC(C)c1ccc(CN)cc1
Mol. weight [g/mol]: 149.23
CAS: 4395-73-7

Physical Properties

Property code	Value	Unit	Source
gf	200.11	kJ/mol	Joback Method
hf	3.84	kJ/mol	Joback Method
hfus	16.98	kJ/mol	Joback Method
hvap	51.05	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.269		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1246.90		NIST Webbook
tb	500.20	K	NIST Webbook
tc	753.77	K	Joback Method
tf	309.66	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.49	J/mol×K	531.95	Joback Method
cpg	331.53	J/mol×K	568.92	Joback Method
cpg	345.68	J/mol×K	605.89	Joback Method
cpg	358.96	J/mol×K	642.86	Joback Method
cpg	371.42	J/mol×K	679.83	Joback Method
cpg	383.09	J/mol×K	716.80	Joback Method
cpg	394.01	J/mol×K	753.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.20	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4395737&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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